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APPLICATION OF FINITE ELEMENT METHOD IN THERMOMECHANICS

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Abstract: *In this paper we consider an application of the finite element method in the field of thermomechanics. We start with a brief presentation of the continuum mechanics balance laws necessary for proper description of material behaviour. Constitutive laws of materials in questions are described. Due to coupled nature of the considered problem we provide a general approach to the coupled problems. Decoupling into several smaller problems is discussed. We propose a general algorithm based on the finite element method capable of dealing with such problem. In addition to the presented theory and procedures, we also provide verification by means of an example.*

Key words: *Engineering Design, Finite Element Method, Thermomechanics, Coupled Problems.*

1. INTRODUCTION

In structural design, mechanical behaviour is of prime importance. However, real situations often involve some accompanying effects. Among them, various thermal effects are most often found. In the most cases, these effects are neglected. But, there are some situations where thermal behaviour must be accounted for.

Numerical approach to such problems can be selected among several choices. Straightforward choice is surely simultaneous solution of thermal and mechanical problem. From the numerical point of view, such approach is probably the most unwanted. Reasons for this lie in the unsymmetrical stiffness matrices and larger system of equations in general. In addition, same time scale must be used in temporal integration of both mechanical and thermal effects. Nevertheless, this procedure cannot be avoided in the case of bifurcation analysis. An alternative to this approach is decoupling the problem into several phases, in this case into mechanical and thermal phase. Advantages of this decoupling are smaller subproblems that are usually symmetrical.

The most often thermal effect is temperature dilatation, i.e. object change dimensions when it is subjected to temperature variations. If these dilatations are constrained, stresses arise proportionally to the constrained dilatations. This situation, in which strains vary linearly with temperature variation is known as linear thermoelasticity. Although a rather simple class of coupled problem, nevertheless it can be classified as coupled problem. These coupling effects take place through influence of thermal field on mechanical field. In linear thermoelasticity it is assumed that mechanical effects do not influence thermal field. Therefore thermal phase can be calculated independently of mechanical one.

2. CONTINUUM MECHANICS FUNDAMENTALS

2.1 Kinematics

We will employ two configurations in order to define various mechanical and thermal fields. In particular, we use referent (initial) configuration that is defined with the initial position of the body in question and current configuration that is defined with the last – current position of the body. In the following text we will denote quantities defined in referent configuration with the upper case symbols, while the quantities in current configuration will be denoted with the lower case symbols (Truesdell & Noll, 1965).

As a fundamental measure of deformation we use a deformation gradient **F**. It is defined as follows:

$$F_{iJ} = \frac{\partial x_i}{\partial X_J} \tag{1}$$

or

$$\mathbf{F} = \mathrm{GRAD}\,\mathbf{x}\,. \tag{2}$$

In above equation x_i and X_i denote positions of a point in the current and initial configuration, respectively. Of a particular interest is also a determinant of deformation gradient:

$$J = \det \mathbf{F} \neq 0\,. \tag{3}$$

This determinant is a measure of volume change. In the isochoric case, i.e. when no volume change take place, it must be:

$$J = 1\,. \tag{4}$$

In the continuum mechanics it is customary to employ various strain tensors. In the current work we use the following strain tensors:

$$\mathbf{C} = \mathbf{F}^t\mathbf{F}\,, \tag{5}$$

which is known as Green or right Cauchy – Green strain tensor and

$$\mathbf{b} = \mathbf{F}\mathbf{F}^t \tag{6}$$

which is known as Finger or left Cauchy – Green strain tensor. These tensors, eq. (5) and eq. (6) are equal to the unit tensor in the case of unloaded body.

2.2 Balance laws

Balance laws of the continuum mechanics will be employed as a basis for the finite element discretization. Therefore, we will provide a brief description of the basic equations in the text that follows.

When the case of thermoplasticity is considered, we must bear in mind that metals subjected to the plastic deformation does not change volume. Consequently, the balance of the mass law must be employed at the some point in the model to enforce condition defined with the eq. (4). This balance law can be written:

$$\frac{\partial}{\partial t}\int_{\upsilon}\rho(x,t)\mathrm{d}\upsilon = 0\,, \tag{7}$$

where $\rho(x,t)$ is known as density function while the integral $\int_{\upsilon}\rho(x,t)\mathrm{d}\upsilon$ is known as the mass of the body. An equivalent relationship that is also often used is:

$$\dot{\rho} + \rho\,\mathrm{div}\,\boldsymbol{\upsilon} = 0\,. \tag{8}$$

Momentum balance defined in current configuration can be stated as follows (Marsden & Hughes, 1994):

$$\frac{\partial}{\partial t}\int_{\phi_t(\mathrm{B})}\rho\boldsymbol{\upsilon}\,\mathrm{d}\upsilon = \int_{\phi_t(\mathrm{B})}\rho\mathbf{b}\mathrm{d}\upsilon + \int_{\partial\phi_t(\mathrm{B})}\mathbf{t}\mathrm{d}s\,. \tag{9}$$

In the above equation $\mathbf{b}(x,t)$ is defined as body forces and $\mathbf{t}(x,t,\mathbf{n})$ is Cauchy stress vector. If the Cauchy stress vector is defined as a force over the surface with the normal $\mathbf{n}$, then it is:

$$\mathbf{t}(x,t,\mathbf{n}) = \boldsymbol{\sigma}(x,t)\cdot\mathbf{n}\,, \tag{10}$$

where $\boldsymbol{\sigma}(x,t)$ is the Cauchy stress tensor. Of further interest is the momentum balance equation written in local form:

$$\rho\dot{\boldsymbol{\upsilon}} = \rho\mathbf{b} + \mathrm{div}\,\boldsymbol{\sigma}\,. \tag{11}$$

The right side of equation

$$\rho\dot{\boldsymbol{\upsilon}} \tag{12}$$

represent inertial forces that are often left out in the static analysis.

The balance of the moment of the momentum leads toward the well-known symmetry property of the Cauchy stress tensor:

$$\frac{\partial}{\partial t}\int_{\phi_t(\mathrm{B})}\rho(\mathbf{x}\times\boldsymbol{\upsilon})\mathrm{d}\upsilon = \int_{\phi_t(\mathrm{B})}\rho(\mathbf{x}\times\mathbf{b})\mathrm{d}\upsilon + \int_{\partial\phi_t(\mathrm{B})}(\mathbf{x}\times\mathbf{t})\mathrm{d}s\,, \tag{13}$$

what yields:

$$\sigma_{ij} = \sigma_{ji}\,. \tag{14}$$

The basis for the thermal part of the model is the balance of energy law:

$$\begin{aligned}\frac{\partial}{\partial t}\int_{\phi_t(\mathrm{B})}\rho\left(e+\frac{1}{2}\boldsymbol{\upsilon}\cdot\boldsymbol{\upsilon}\right)\mathrm{d}\upsilon &= \int_{\phi_t(\mathrm{B})}\rho(\mathbf{b}\cdot\boldsymbol{\upsilon}+\boldsymbol{r})\mathrm{d}\upsilon + \\ &+ \int_{\partial\phi_t(\mathrm{B})}(\mathbf{t}\cdot\boldsymbol{\upsilon}+\boldsymbol{h})\mathrm{d}s\end{aligned}\,, \tag{15}$$

where $r(x,t)$ represent heat input per unit mass, $e(x,t)$ internal energy per unit mass, $h(x,t,\mathbf{n})$ heat flux on surface with normal $\mathbf{n}$. Heat flux vector is defined as:

$$\boldsymbol{h}(x,t,\mathbf{n}) = -\mathbf{q}(x,t)\cdot\mathbf{n}\,, \tag{16}$$

where

$$\mathbf{q} = -k\nabla\theta \tag{17}$$

is the Kirchhoff heat conduction law.

Balance of energy law can be also written using current configuration:

$$\rho\dot{e} + \mathrm{div}\,\mathbf{q} = \boldsymbol{\sigma}\cdot\mathbf{d} + \rho r\,. \tag{18}$$

Some restrictions are enforced by the second law of the thermodynamics or Clausius – Duhem inequality written in initial configuration:

$$\frac{\partial}{\partial t}\int_{\phi_t(\mathrm{B})}\rho\eta\mathrm{d}\upsilon \geq \int_{\phi_t(\mathrm{B})}\frac{\rho r}{\theta}\mathrm{d}\upsilon + \int_{\partial\phi_t(\mathrm{B})}\frac{\mathbf{h}}{\theta}\mathrm{d}a\,. \tag{19}$$

where

$$\eta = \frac{\partial e}{\partial\theta} \tag{20}$$

is specific entropy.

If internal entropy production per unit mass γ is introduced, following form of the inequality is obtained:

$$\gamma \equiv \dot{\eta} - \frac{r}{\theta} + \frac{1}{\rho\theta}\mathrm{div}\,\mathbf{q} - \frac{\mathbf{q}}{\rho\theta^2}\cdot\mathrm{grad}\,\theta \geq 0\,, \tag{21}$$

what can be further transformed to:

$$\left.\begin{aligned}\gamma_{\mathrm{loc}} &= \dot{\eta} - \frac{r}{\theta} + \frac{1}{\rho\theta}\mathrm{div}\,\mathbf{q} \geq 0\\ \gamma_{\mathrm{con}} &= -\frac{\mathbf{q}}{\rho\theta^2}\cdot\mathrm{grad}\,\theta \geq 0\end{aligned}\right\}, \tag{22}$$

where γ_{loc} is local entropy production and γ_{con} is entropy production due to heat conduction. First inequality corresponds to the fact that body with homogeneous temperature field without heat sources can absorb mechanical energy but cannot return it. Second inequality constrains heat flow from the warmer to colder bodies and does not allow opposite processes (Simo & Miehe, 1992).

Presented balance laws as well as basic kinematics should be augmented with constitutive laws in order to complete the proposed thermomechanical model.

2.3 Constitutive laws

Stresses are calculated from free energy function:

$$\mathbf{S} = 2\frac{\partial\psi}{\partial\mathbf{C}}\,. \tag{23}$$

This means that the structure of the free energy function is determined by the material behaviour. Several choices are available at this point.

In the case of linear, uncoupled thermoelasticity free energy is given by (Boley & Wiener, 1967):

$$\psi = T(\theta) + M(J,\theta) + U(J,\theta) + W\left(\overline{\mathbf{b}}^e,\theta\right), \tag{24}$$

where are:

- $T(\theta)$ - thermal potential,
- $M(J,\theta)$ - thermoelastic coupling,
- $U(J)$ - volumetric potential,
- $W(\mathbf{C})$ - deviatoric potential.

The specific form for above potentials can take different forms depending on the material. For the specific case of the most metals, they are usually taken to be:

thermal potential:

$$T(\theta) = \rho_0 c_0\left[(\theta-\theta_0) - \theta\ln\frac{\theta}{\theta_0}\right], \tag{25}$$

thermoelastic coupling potential:

$$M(J,\theta) = (\theta-\theta_0)[-3\alpha\,\partial_J U(J,\theta)], \tag{26}$$

volumetric potential:

$$U(J) = \frac{1}{2}\kappa\left[\frac{1}{2}\left(J^2-1\right) - \ln J\right] \tag{27}$$

and deviatoric potential:

$$W(\mathbf{C}) = \frac{1}{2}\mu\left[\mathrm{tr}\left(\overline{\mathbf{C}}\overline{\mathbf{C}}^{p^{-1}}\right) - 3\right]. \tag{28}$$

Above we do not consider change of material parameters with temperature.

In the case of coupled thermoplasticity constitutive law must account for hardening. Hardening can be of isotropic and kinematic type, or a combination of these two. Several possible choices for these hardening models have been proposed.

In addition to finite strain modeling in the case of thermoplasticity, a general model should consider a temperature dependency of all material parameters. In this case we propose the following form for the free energy function:

$$\psi = T(\theta) + M(J,\theta) + U(J,\theta) + W\left(\overline{\mathbf{b}}^{e},\theta\right) + K(\xi,\mathbf{z},\theta)\,. \tag{29}$$

In the above equations it is:
thermal potential:

$$T(\theta) = -\int_{\theta_0}^{\theta} d\overline{\theta} \int_{\theta_0}^{\overline{\theta}} \rho_0 c_0\left(\hat{\theta}\right)\frac{d\hat{\theta}}{\hat{\theta}}\,, \tag{30}$$

what means that specific heat capacity should be defined as:

$$c = -\theta\,\partial^2_{\theta\theta}\psi = c_0(\theta) - \theta\,\partial^2_{\theta\theta}(M + U + W + K)\,, \tag{31}$$

thermoelastic coupling potential:

$$M(J,\theta) = (\theta - \theta_0)\left[-3\alpha(\theta)\partial_J U(J,\theta)\right], \tag{32}$$

volumetric potential:

$$U(J,\theta) = \frac{1}{2}\kappa(\theta)\left[\frac{1}{2}\left(J^2 - 1\right) - \ln J\right], \tag{33}$$

deviatoric potential:

$$W\left(\overline{\mathbf{b}}^{e},\theta\right) = \frac{1}{2}\mu(\theta)\left[\mathrm{tr}\left(\overline{\mathbf{b}}^{e}\right) - 3\right], \tag{34}$$

and hardening potential:

$$\left.\begin{aligned} K(\xi,\mathbf{z},\theta) &= \frac{1}{2}h(\theta)\xi^2 + \left[y_0(\theta) - y_\infty(\theta)\right]H(\xi) + \\ &+ \frac{1}{2}h_{kin}(\theta)\mathrm{tr}[\mathbf{z}] \\ H(\xi) &= \begin{cases} \xi - \dfrac{\left(1 - e^{-\delta\xi}\right)}{\delta}, & \text{for } \delta \neq 0 \\ 0 & \text{for } \delta = 0 \end{cases} \end{aligned}\right\}. \tag{35}$$

We also use von Mises yield criterion of the following form:

$$\phi(\boldsymbol{\tau},\beta,\boldsymbol{\alpha},\theta) = \left\|\mathrm{dev}\,\boldsymbol{\tau} - \mathrm{dev}\,\boldsymbol{\alpha}\right\| + \sqrt{\frac{2}{3}}\left[\beta - \sigma_y(\theta)\right] \leq 0\,. \tag{36}$$

This criterion defines elastic domain as the interior of this surface and boundary as plastic domain.
In addition to this constitutive model in the thermoplasticity we also employ multiplicative decomposition of the deformation gradient into the elastic and plastic part (Simo & Hughes, 1998):

$$\mathbf{F} = \mathbf{F}^e\mathbf{F}^p\,. \tag{37}$$

Elastic part of deformation gradient represents deformation from the stress-free intermediate configuration to the current configuration, Fig. 1.

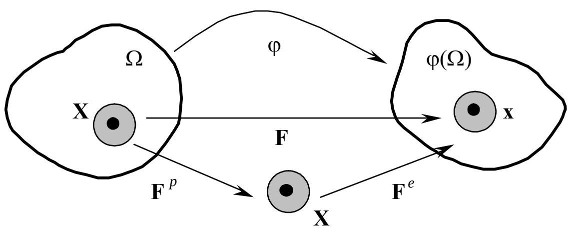

Fig. 1. Multiplicative decomposition of the deformation gradient

3. SOME ASPECTS OF THE NUMERICAL PROCEDURE

As already stated in the introduction, thermomechanical problems are coupled. In this work we will choose to decouple the problem into two steps: mechanical and thermal step. As a consequence, stiffness matrix is no longer unsymmetrical and with lower rank. Therefore, we can use more efficient numerical procedures. However, the resulting scheme is no longer unconditionally stable. Luckily, this is not of importance for the thermoplasticity of metals. Unconditional stability can be achieved by the application of the so-called isentropic split. The basic property of such approach is separation in two phases: one with constant entropy and one where entropy is allowed to change.
Mechanical and thermal step are linearized in order to obtain algorithmically consistent tangent stiffness matrices. Since we use Newton-Raphson scheme to deal with nonlinearities, such linearization is essential condition to obtain quadratic convergence typically associated with this scheme. Obtained stiffness matrix for the mechanical phase consists of the following parts:

$$\mathbf{K}_M = \mathbf{K}_{Mgeo} + \mathbf{K}_{Mmat} + \mathbf{K}_{ML}\,, \tag{38}$$

where parts are geometrical stiffness, material stiffness and follower forces part, respectively. Geometrical stiffness accounts for large displacement effects, material stiffness nonlinearities due to nonlinear material behaviour and the follower forces part considers variations in load due to geometry change.
As a numerical tool, we employ the finite element method (Zeinkiewicz & Taylor, 2000; Hughes, 2000). Primary fields to solve are taken as usual: displacement and temperature. However, as it is well known, plasticity of metals exhibit volume constancy. This leads toward problems in the numerical procedure – to the so-called locking behaviour which is characterized by the inability to properly model pressure part of the stress tensor. In order to circumvent such problems, we introduce an additional pressure field.
For the numerical modeling of plasticity we used radial return method. Stresses are predicted as elastic and then if obtained state lies outside the yield surface is projected – corrected to lie on the yield surface.

4. EXAMPLE

In this example we consider behaviour of cylindrical specimen under axial load. This is the well-known uniaxial test. Specimen is 53.334 mm long and radius is 6.413 mm. Due to the axial symmetry of the specimen, only one quarter of the longitudinal section of the specimen is actually discretized by the 200 isoparametric finite elements.
Calculation has been carried out with 200 equal time steps.
Thermal boundary conditions allowed heat convection into the environment. Convection heat coefficient was $h = 17{,}5\cdot 10^{-3}$ N/mmsK. Environment temperature was constant and equal to $\theta_0 = 293\,\mathrm{K}$.
Experimentally noticed behaviour is characterized by the occurrence of the so-called neck at the position of the eventual breaking of the test specimen. If this process is modeled as isothermal, then one needs to introduce an imperfection to initiate necking. However, it is to be emphasized that with presented thermoplastic model imperfection is no longer needed. Nonhomogenities that arise in the temperature field are trigger for the necking behaviour.

We consider the following material properties for the specimen:

Quantity	Symbol	Value
Shear modulus	μ	164206 MPa
Bulk modulus	κ	80193.8 MPa
Initial yield stress	y_0	450 MPa
Isotropic hardening modulus	h	129.24 MPa
Saturation hardening modulus	$y_{0,\infty}$	715 MPa
Hardening exponent	δ	16.93
Density	ρ	$7{,}8 \cdot 10^{-9}$ Ns^2/mm^4
Thermal expansion coef.	α	$1{,}0 \cdot 10^{-5}$ K^{-1}
Thermal conduction	k	45 N/sK
Heat capacity	c_0	3.588 N/mm^2K
Dissipation factor	χ	0.9
Yield stress softening	ω_0	0,002 K^{-1}
Hardening modulus softening	ω_h	0,002 K^{-1}

Table 1. Thermoplastic material properties of the uniaxial test specimen

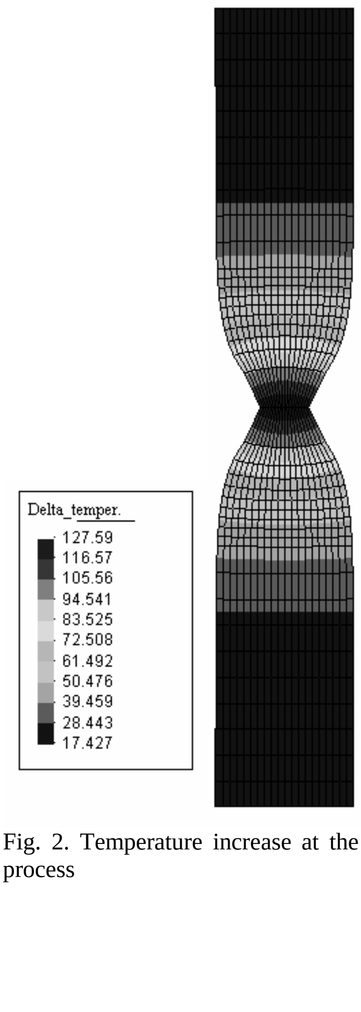

Fig. 2. Temperature increase at the end of the stretching process

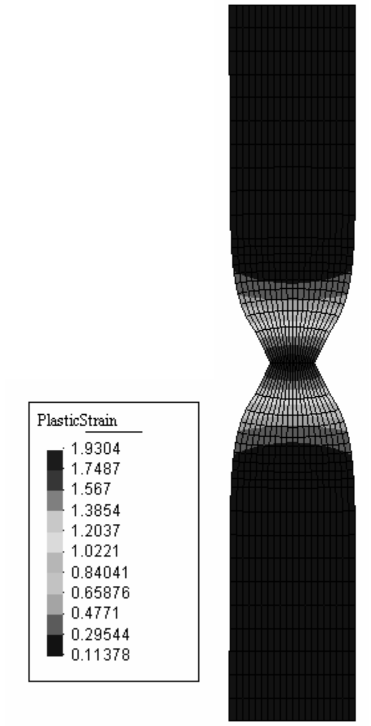

Fig. 3. Equivalent plastic strain at the end of the process

5. CONCLUSION

In the engineering design thermomechanical problems are frequent. We presented fundamentals of these problems. Although several different aspects of the thermomechanical problems are addressed, an emphasis on finite strain thermoplasticity is given. An example that is computationally intensive has been presented. However, a lot of other possible modifications to the presented procedure can be introduced. For example, strain rate dependency can be added to model thermoviscoplastic behaviour. In addition, damage models, micro – macro coupling and other effects can be introduced.

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